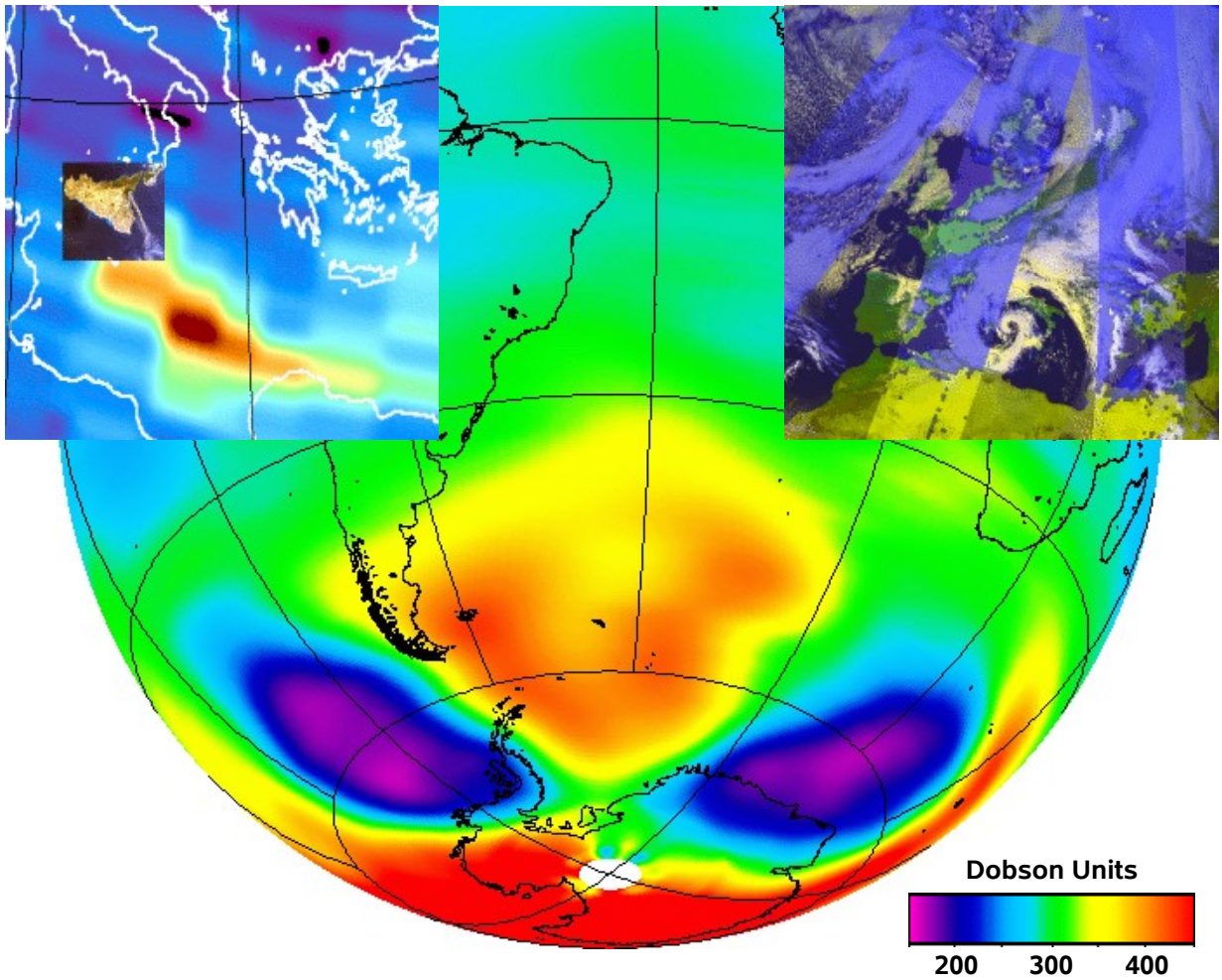
Product User Manual for GOME Total Columns of Ozone, Minor Trace Gases, and Cloud Properties

(O3M-SAF OTO and NTO)



Doc. No: DLR/GOME/PUM/01
Iss./Rev.: 2/A
Date: 28 January 2009

Deutsches Zentrum für Luft und Raumfahrt e.V. – DLR
Oberpfaffenhofen, Germany

Signatures

Action: Name	*Affiliation*	*Function*	*Date*	*Signature*
prepared by: D. Loyola R. W. Zimmer S. Kiemle P. Valks T. Ruppert	 DLR-MF DLR-MF DLR-DFD DLR-MF DLR-DFD	 GOME Project Manager GOME Project Engineer DIMS Project Manager GOME Project Scientist GOME Project Engineer	28 January 2009	
BUFR v3 by: L. Butenko	former DLR-MF	GOME Project Engineer	14 June 2006	
HDF5 by: Y. Livschitz	former DLR-MF	GOME Project Engineer	1 November 2004	
released by: D. Loyola R.	DLR-MF	GOME Project Manager	28 January 2009	

Distribution List

Function	*Organization*
UPAS Team	DLR-MF, DLR-DFD
GOME/ERS-2 Team	ESA, BIRA, RTS, AUTH, various
O3M-SAF Team	EUMETSAT, FMI, AUTH, BIRA, KNMI, various

Document Change Log

Issue	*Rev*	*Date*	*Section*	*Description of Change*
1	A	31 July 2004 to 20 July 2006	all	HDF5 and BUFR output product format documents merged in this product user manual
1	B	5 October 2006	4, 5	Content of chapters added
1	C	10 November 2006	all	First official version of this document
1	D	6 March 2007	5.7 6.2, 6.5	Fix file name convention Added VCDQualityIndicator, QualityFlags, CloudMode, CloudType, AMFTotal, AMFTotal_Error, OrbitActualDuration, new receiving stations
1	E	30 April 2008	all 6 7	Revised following ORR-A Added in HDF5 section: - IterativeVCDNumberOfIterations - a-priori O3_Profile - T_Profile BUFR product update to BUFR version 4
2	A	9 December 2008 28 January 2009	all 6	Revised following ORR-B Finalized HDF5 product format: - Moved trace gas specific datasets into own groups inside DETAILED_RESULTS - Moved cloud properties into own group

Table of Contents

1 Introduction....7
1.1 Purpose and Scope....7
1.2 References....9
1.2.1 Applicable Documents....9
1.2.2 Reference Documents....9
1.3 Abbreviations and Acronyms....10
2 GOME Instruments....11
2.1 Introduction....11
2.2 GOME/ERS-2....12
2.3 GOME-2/MetOp....12
2.4 Measurement Scenarios, Timelines and Instrument Modes....13
3 Algorithm Description....14
3.1 Summary....14
3.2 Trace Gas and Cloud Products....14
4 Processing....15
4.1 GOME/ERS-2....15
4.2 GOME-2/MetOp....15
4.3 Data Management....16
4.4 Quality Control and Monitoring....16
4.5 Geophysical Validation....17
4.6 User Services....17
5 Total Column Trace Gases and Cloud Products....18
5.1 Units....18
5.2 Geographical Coverage and Granularity....18
5.3 Spatial Resolution....18
5.4 Delivery Time....18
5.5 Expected Accuracy....19
5.6 Product Formats....19
5.7 File Name....20
5.8 Product Dissemination....21
5.8.1 GOME/ERS-2....21
5.8.2 GOME-2/MetOp....21
5.9 Product Ordering....22
5.9.1 GOME/ERS-2....22
5.9.2 GOME-2/MetOp....22
6 HDF5 Product Format Description....23
6.1 Structure....24
6.1.1 Description of Common Items....25
6.2 META_DATA Group....26
6.3 GEOLOCATION Group....29

6.4 TOTAL_COLUMNS Group....31
6.5 CLOUD_PROPERTIES Group....32
6.6 DETAILED_RESULTS Group....33
6.6.1 DETAILED_RESULTS/O3 Subgroup....34
6.6.2 DETAILED_RESULTS/NO2 Subgroup....34
6.6.3 DETAILED_RESULTS/SO2 Subgroup....35
6.7 Detailed Flag Description....35
6.7.1 QualityFlags....35
6.7.2 NO2Tropo_Flag....36
6.7.3 SO2_Flag....36
7 BUFR Product Format Description....37
7.1 Structure....37
7.2 Section 0 - Indicator Section....38
7.3 Section 1 - Identification Section....38
7.4 Section 3 - Indicator Section....38
7.5 Section 3 - UPAS Level-2 Specific List of Descriptors....39
7.6 Section 4 - Indicator section....40
7.7 Section 5 - End Section....40
7.8 Trace Gas Table....40
A Appendixes....41
A.1 HDF5 Data Types....41
A.2 Traceability Matrix of HDF5 Metadata to EECF Parameters....42
A.3 Traceability Matrix of HDF5 Metadata to UMARF Parameters....43

1 Introduction

1.1 Purpose and Scope

DLR has been producing on an operational basis a range of total column trace gases and cloud products for GOME/ERS-2 in the framework of ESA's D-PAF project. In the same way, DLR produces total column trace gases and cloud products for GOME-2/MetOp in the framework of EUMETSAT's O3M-SAF.

DLR has a long experience in operational processing of GOME data and has developed a generic software for this purpose: the Universal Processor for UV/VIS Atmospheric Spectrometers (UPAS) [A1] system. This document is the user manual for the GOME/ERS-2 and GOME-2/MetOp total column trace gases and cloud products available at DLR.

In this document, the terms GOME/ERS-2 and GOME-2/MetOp are used to reference the specific instruments. The general term GOME applies to both sensors.

The trace gases total column products are:

- Ozone (O_3) total column
- NO_2 total column
- BrO total column
- H_2O total column
- SO_2 total column
- HCHO total column
- OClO total column

The trace gases tropospheric column products are:

- NO_2 tropospheric column
- Ozone tropospheric column

Additionally DLR provides the following cloud properties derived from GOME measurements:

- Cloud fraction
- Cloud-top albedo (optical thickness)
- Cloud-top height (pressure)

DLR provides near-real-time (NRT), off-line (OL), and reprocessed products. The NRT products have the same granularity as the input GOME data (i.e. downlink or PDU) and

are made available and disseminated to the users within 2 hours 30 minutes of sensing. The OL products are consolidated orbits from ascending node crossing to ascending node crossing and are available and disseminated to the users two weeks (up to four weeks in case of GOME/ERS-2) after sensing. Additionally, DLR provides reprocessed products for climate applications; the complete GOME/ERS-2 data record has been reprocessed and validated every two to three years using improved algorithms.

GOME/ERS-2 and GOME-2/MetOp provide a unique data record of atmospheric measurements covering a time frame of around 25 years. DLR together with the partner organizations ESA and EUMETSAT will assure the continuity between GOME/ERS-2 and GOME-2/MetOp total column products. In this framework it is important to provide to the users a unified data format for accessing the GOME products. The “Hierarchical Data Format” (HDF) and the “Binary Universal Form for the Representation of meteorological data” (BUFR) have been selected for the GOME total column products. HDF and BUFR are self-describing, machine-independent file formats commonly used for storage and transfer of scientific and meteorological data.

The present document is divided into the following sections:

- Overview of the GOME/ERS-2 and GOME-2/MetOp instruments including instrument modes
- Summary of the algorithms used for the retrieval of trace gases total columns and cloud properties
- Summary of the processing steps
- Product description including the used HDF5 and BUFR format
- Appendixes

1.2 References

1.2.1 Applicable Documents

[A1] Design Document for the GOME-2 Universal Processor for Atmospheric Spectrometers, SAF/O3M/DLR/DD/001, Issue 2.0, October 2003

[A2] EECF to PAF Interface Specifications, ER IS EPO GE 0102, Issue 3.0, January 1990

[A3] UMARF to SAFs Interface Control Document, EUM/UMA/ICD/004, Issue 3.12, April 2006

[A4] Product Requirements Document, SAF/O3M/FMI/RQ/PRD/001, Rev. 06, May 2008

1.2.2 Reference Documents

[R1] "Algorithm Theoretical Basis Document for GOME-2 Total Column Products of Ozone, Minor Trace Gases, and Cloud Properties (GDP 4.2 for O3M-SAF OTO and NTO)", DLR/GOME-2/ATBD/01, Iss./Rev. 2/A, January 2009.

[R2] "Algorithm Theoretical Basis Document for GOME Total Column Densities of Ozone and Nitrogen Dioxide, UPAS/GDOAS: GDP 4.0", ERSE-DTEX-EOPG-TN-04-0007, Iss./Rev. 1/A, December 2004

[R3] "Delta Validation Report for ERS-2 GOME Data Processor upgrade to version 4.0", ERSE-CLVL-EOPG-TN-04-0001, Iss./Rev. 1.0, December 2004

[R4] "Product Specification Document of the GOME Data Processor", ER-PS-DLR-GO-0016, Iss./Rev. 4/B, December 2004

[R5] "GOME-2 Level 1 Product Format Specification", EPS/MIS/SPE/97232, March 2004

[R6] "GOME-2 Products Guide", EUM/OPS-EPS/MAN/05/0005, Issue 1.0, February 2005

[R7] HDF5 File Format Specification, http://hdf.ncsa.uiuc.edu/HDF5/doc/H5.format.html

[R8] BUFR Format Specification, http://www.wmo.ch/web/www/WDM/Guides/Guide-binary-1A.html

1.3 Abbreviations and Acronyms

A list of abbreviations and acronyms used throughout this document is given below:

AAIA	Absorbing Aerosol Indicator Algorithm
AMF	Air Mass Factor
BIRA-IASB	Belgian Institute for Space Aeronomy
BUFR	Binary Universal Form for the Representation of meteorological data
CCSDS	Consultative Committee for Space Data Systems
DLR	Deutsches Zentrum für Luft- und Raumfahrt e.V. (German Aerospace Centre)
DOAS	Differential Optical Absorption Spectroscopy
D-PAF	German processing and archiving facility
DU	Dobson Unit
EPS	EUMETSAT Polar System
ERS-2	European Remote Sensing Satellite-2
ESA	European Space Agency
ESC	Effective Slant Column
EUMETSAT	European Organisation for the Exploitation of Meteorological Satellites
GDOAS	GODFIT-DOAS
GDP	GOME Data Processor
GOME	Global Ozone Monitoring Experiment
HDF	Hierarchical Data Format
IMF	Remote Sensing Technology Institute
MetOp	Operational Meteorological Satellite
NRT	Near Real Time
NTO	Identifier used for near-real-time total column trace gas products
O3M-SAF	SAF on Ozone and Atmospheric Chemistry Monitoring
OL	Off-line
OTO	Identifier used for offline total column trace gas products
PDU	Product Dissemination Unit
PMD	Polarisation Measurement Device
RMS	Root Mean Square
SAF	Satellite Application Facility
SZA	Solar Zenith Angle
TBD	To be Defined
TOA	Top of Atmosphere
UMARF	Unified Meteorological Archiving and Retrieval Facility
UV	Ultra Violet
UPAS	Universal Processor for UV/VIS Atmospheric Spectrometers
UTC	Universal Time Coordinate
VCD	Vertical Column Density
VIS	Visible

2 GOME Instruments

2.1 Introduction

The Global Ozone Monitoring Experiment (GOME) is a scanning spectrometer that captures light reflected from the Earth's surface and atmosphere. The spectrometer splits the light into its spectral components covering the UV/VIS region from 240 nm to 790 nm at a resolution of 0.2 nm to 0.4 nm.
The measured spectra are mainly used to derive ozone total column and vertical profile, nitrogen dioxide, bromine oxide, water vapour, oxygen, sulphur oxide and other trace gases, as well as cloud properties and aerosols.
The next figure shows a schematic representation of GOME optical layout. A scan mirror (26) directs the light emitted from the Earth's atmosphere or the Sun diffuser (24) into the instrument. The spectrometer splits incoming light into four channels (11, 12, 18, 19) using a complex array of telescopes (5, 25), prisms (4, 6) and gratings (8, 9, 20, 21). Detectors at the end of each optical path (13 to 16) collect information about the signal in each channel.

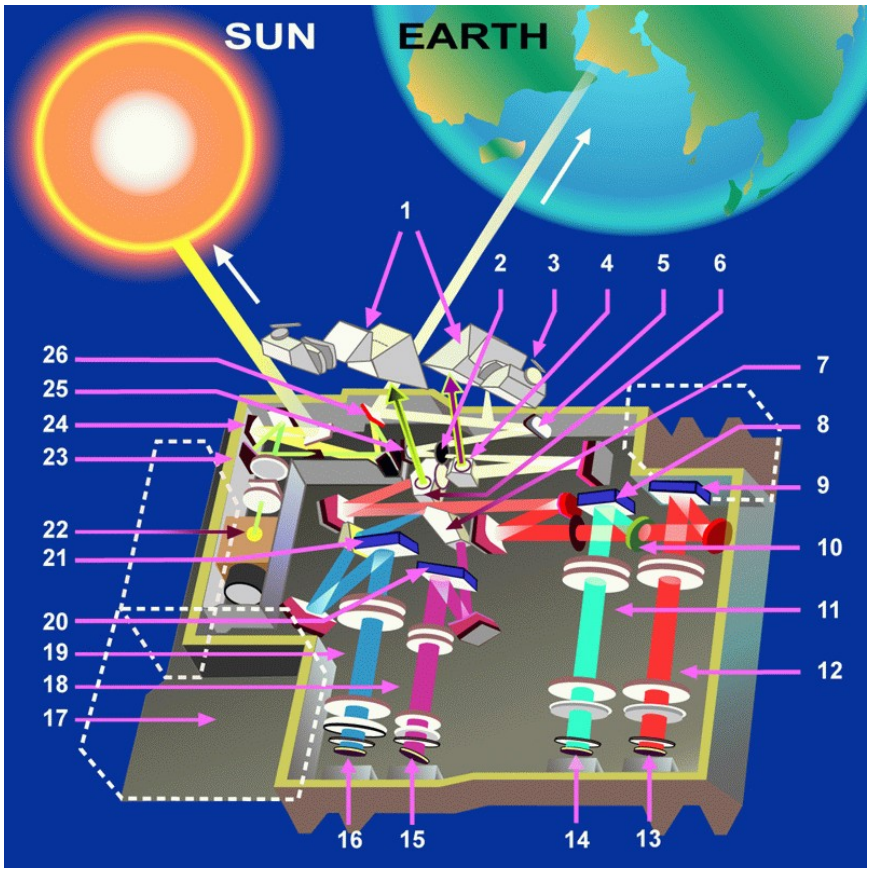


Figure 1: GOME optical layout (courtesy of ESA/ESTEC)

2.2 GOME/ERS-2

In June 1990, the ESA Council approved the satellite project to follow the first European Remote Sensing Satellite (ERS-1). The ERS-2 satellite was intended to provide data continuity between ERS-1 and the European polar platforms. ERS-2 was launched on 21 April 1995.
In addition to the ERS-1 mission objectives, ERS-2 was scheduled to make a significant contribution to atmospheric chemistry. To meet this need, ERS-2 carried GOME, an instrument designed to measure a range of atmospheric trace constituents in the troposphere and stratosphere.
GOME/ERS-2 is a nadir viewing spectrometer, which in its normal mode scans across track in three steps. The field of view of each step may be varied in size from 40 km x 40 km to 320 km x 40 km, with five options allowed. The mode with the largest footprint (three steps with a total coverage of 960 km x 40 km) provides global coverage at the equator within 3 days.
DLR developed the GOME Data Processor (GDP) system, the operational ground segment for GOME/ERS-2. GDP incorporates a Level 0-to-1 processing chain, the complete GOME/ERS-2 data archive, a DOAS-based total column retrieval process (Level 1-to-2), and processing chain for the generation of value added products.

2.3 GOME-2/MetOp

On 30 January 1998, the ESA Earth Observation Programme Board gave its final go-ahead for the MetOp Programme. The instruments on the MetOp satellites are designed to produce high-resolution images of the Earth's surface, vertical temperature and humidity profiles, and temperatures of the land and ocean surface on a global basis. In addition, there are instruments for monitoring trace gases and wind flow over the oceans. This instrument payload is of significant value to meteorologists and other scientists, particularly to those studying the global climate.
Given the need for global-scale routine monitoring of the abundance and distribution of ozone and associated trace gas species, a proposal was put forward for the inclusion of GOME-2 on the MetOp satellites. MetOp-A was launched on 19 October 2006 as part of the Initial Joint Polar System (IJPS) in co-operation with NOAA in the USA.
The GOME-2/MetOp field of view of each step may be varied in size from 5 km x 40 km to 80 km x 40 km. The mode with the largest footprint (twenty four steps with a total coverage of 1920 km x 40 km) provides daily near global coverage at the equator [R6].
Based on the successfully work with the GOME Data Processors, the German Aerospace Centre (DLR) plays a major role in the design, implementation and operation of the GOME-2/MetOp ground segment for total column products. DLR is a partner in the Satellite Application Facility on Ozone and Atmospheric Chemistry Monitoring (O3M-SAF), which is part of the Eumetsat Polar System (EPS) ground segment, and is responsible in this project for the generation of total column amounts of the various trace gases and cloud properties which may be retrieved from GOME-2/MetOp level 1b products.

2.4 Measurement Scenarios, Timelines and Instrument Modes

GOME/ERS-2 and GOME-2/MetOp follow in general the same operational scenarios, see

- http://gome.eumetsat.int
- http://www.eumetsat.int/EPSCalValExtranet/Main/GOMECalVal/index.htm

for more details.

- Earth Observation Mode

  This mode includes nadir/narrow/static/north-polar/south-polar scanning measurements with various integration times depending on solar zenith angle. This is the default mode for the day side. Only the data acquired in this mode are used for geophysical retrievals.

- Calibration Modes

  This mode includes Sun/Moon/dark/spectral-light/LED/white-light measurements. Most of this calibrations are performed on the night side.

The effective optical throughput and the potential data rate for GOME-2/MetOp are much higher than those for GOME/ERS-2[1]. The default integration times for GOME-2/MetOp is 4 to 8 times smaller than those for GOME/ERS-2.

1 The effective optical throughput is enhanced by approximately a factor of 2, and co-adding (as used for GOME/ERS-2) is not required because of the higher data rate (10 times faster).

3 Algorithm Description

3.1 Summary

The GOME Data Processor (GDP) operational algorithm is the baseline algorithm for the trace gas column retrievals from GOME/ERS-2 and GOME-2/MetOp. The latest GDP 4.x uses an optimised DOAS (Differential Optical Absorption Spectroscopy) algorithm to determine the trace gas slant column. The DOAS slant column fitting is followed by Air Mass Factor (AMF) conversions to generate vertical columns. Cloud information used in the trace gas retrieval is obtained with the OCRA and ROCINN algorithms. A detailed description of the GDP algorithm is given in [R1] and [R2].

3.2 Trace Gas and Cloud Products

The GOME/ERS-2 and GOME-2/MetOp trace gas column densities and cloud properties (level-2 product) are retrieved from GOME (ir)radiance and PMD data (level-1 product). The following table lists the trace gas column and cloud products provided by DLR, and the corresponding wavelength regions used for the retrieval.

Product	*Wavelength region (nm)*
O_3 column	325.0-335.0
NO_2 column	425.0-450.0
BrO column	336.0-351.5
SO_2 column	315.0-326.0
H_2O column	611.0-700.0
HCHO column	337.5-359.0
OClO column	365.0-389.0
Cloud fraction	300-800 (PMD-p)
Cloud-top height (pressure) and albedo (optical thickness)	758-771

4 Processing

The Universal Processor for UV/VIS Atmospheric Spectrometers (UPAS) is the core GOME retrieval system at DLR [A1]. UPAS is a new-generation Level 2 system for the processing of operational near-real-time and off-line trace gas and cloud properties products. UPAS takes as input the calibrated and geolocated Level 1 radiances from different sensors (e.g. GOME/ERS-2 and GOME-2/MetOp) and produces total columns of trace gases (e.g. O_3, NO_2, BrO, H_2O, SO_2, HCHO and OClO) and cloud properties (cloud fraction, cloud-top albedo and height).
The UPAS system is based on a scalable client/server architecture, which makes it possible to run the system with an unlimited number of processing nodes. The average UPAS processing time for O_3, NO_2, and cloud retrieval includes ~15% on pre-processing tasks, ~15% on DOAS, ~60% on explicit calls to the radiative transfer model LIDORT for AMF calculations, and the rest on Level 1 loading and other tasks. The reprocessing of one year of GOME/ERS-2 data can be done in just one day using 10 processing cores.

4.1 GOME/ERS-2

DLR has a processing chain for GOME/ERS-2 NRT and OL total column products that is being used operationally since 1995. It includes data ingestion, from level 1 to level 4 product generation, quality control, product archiving, data dissemination, and ordering.

4.2 GOME-2/MetOp

DLR has developed the operational processing chain for GOME-2/MetOp total column products. The level 1b products are generated at the EPS ground segment in EUMETSAT [R6] and received at DLR via EUMETCast. DLR generates GOME-2/MetOp level 2 total column and cloud products using UPAS.
There are different modules for quality control and monitoring, production control, archiving and order handling. The level 2 products generated at DLR are validated on a regular basis by the O3M-SAF partner institutes AUTH, BIRA, FMI and KNMI. The GOME-2/MetOp level 2 NRT products are disseminated primary with EUMETCast and internet. The off-line products are disseminated via Internet and media. The ordering of products can be done via dedicated user services.
The GOME-2/MetOp level 1 products are delivered in NRT (approx. 1:45 hours after sensing) to the user community via EUMETCast. The NRT level 1 products are delivered in so called PDU files (product dissemination unit) containing 3 minutes of measurements. The ground-segment at DLR needs less than 15 minutes for acquiring the input data, retrieving the trace gas total columns and disseminating the resulting products (Figure 2), that means the GOME-2/MetOp total column products are available in less than 2 hours after sensing.
The GOME-2/MetOp operational system for NRT processing comprises two 64-bit Linux PCs under a high reliability configuration, and several double dual core 64-bit Linux PCs for OL processing.

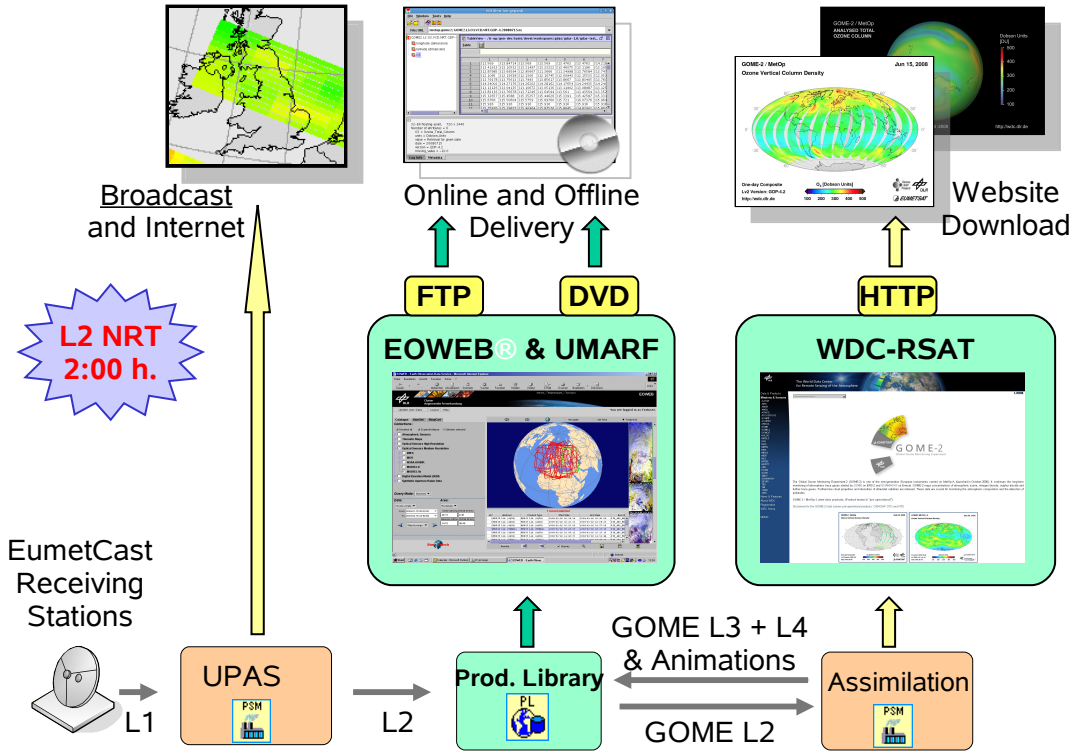


Figure 2: GOME-2/MetOp processing chain

4.3 Data Management

The processing of GOME-2/MetOp data is embedded in DLR's multi-mission facility ensuring high availability and sustainability. The German National Remote Sensing Data Library stores the data for the long-term enabling monitoring of global change and data reprocessing based on enhanced methodology.
Information and data of O3M-SAF products generated at DLR are disseminated through different channels: through direct FTP-push to authorized users and through the EUMETCast broadcast system for near-real-time users, through the EUMETSAT user services and by individual ordering and delivery through DLR's on-line user services EOWEB® (Figure 2).

4.4 Quality Control and Monitoring

The quality of the OL products is controlled before they are archived and disseminated to the users. A dedicated quality control tool integrated into DLR's data management system displays a set of parameters generated automatically by UPAS for each processed orbit.
The quality control tool performs limit checks and computes some statistics to show the confidence levels of the product and its evolution within time. DLR experts examine the displayed parameters and set the corresponding quality stamp only for the off-line product.

4.5 Geophysical Validation

The geophysical validation of the official GOME products is performed by independent partner organizations: AUTH, BIRA, FMI and KNMI. The validation is accomplished using ground-based measurements available through the World Ozone and Ultraviolet radiation Data Centre, ground-based measurements from the NDACC network, other satellite data, as well as data assimilation techniques. The validation results are publicly available on the internet, see section 5.9.

4.6 User Services

Information about data and services are accessible through the websites given in section 5.9.
The interactive catalogue and ordering interface EOWEB® from DLR allows individual product searches and ordering.
Catalogue information from the O3M-SAF products generated at DLR are regularly made available to the central EUMETSAT facility UMARF. The users can query the catalogue of the UMARF and submit their request, the UMARF facility will then send to each SAFs orders requested by the end users about SAF products catalogued in UMARF. DLR's data management system will then deliver the requested products to the user.
DLR operates additionally on-line user services on remote sensing data in the framework of the World Data Center for Remote Sensing of the Atmosphere (WDC-RSAT http://wdc.dlr.de), allowing additionally access to the GOME-2/MetOp value added products produced at DLR (http://wdc.dlr.de/sensors/gome2, left side of Figure 2).

5 Total Column Trace Gases and Cloud Products

The level 2 total column products generated with the UPAS system contain retrieved trace gas vertical columns and cloud properties, as well as other geophysical parameters; corresponding errors on these quantities, and a number of additional diagnostics, quality flags and intermediate results.

5.1 Units

Dataset	Units
Total ozone and SO_2 column amount	Dobson Units [DU]
Other trace gas column amounts	[mol.cm^{-2}]
Cloud fraction and cloud-top albedo (optical thickness)	(unitless) [-]
Height	[km]
Pressure	[hPa]
Angles are given at Top-of-Atmosphere (70 km)	[0 to 360 degrees]
Geographical Coordinates	longitude [0 to 360 degrees] latitude [–90 to +90 degrees]
Errors	relative values [%]

5.2 Geographical Coverage and Granularity

GOME/ERS-2 has a nominal global coverage at the equator after three days. GOME-2/MetOp has a daily near global coverage at the equator. Depending on the scanning mode used, the measured ground pattern may be different.
The NRT, operational OL and reprocessed products have by default a global coverage. The coverage of trace gases available only under special conditions may be reduced, e.g. SO_2 measured during volcanic eruption.
The NRT products have the same granularity as the downlink or PDU. The OL and reprocessed products are consolidated orbits from ascending node to ascending node.

5.3 Spatial Resolution

GOME/ERS-2 has three forward-scan pixels with a nominal resolution of 40 km x 320 km, and one back-scan pixel with a nominal resolution of 40 km x 960 km.
GOME-2/MetOp has 24 forward-scan pixels with a nominal resolution of 40 km x 80 km, and 8 back-scan pixels with a nominal resolution of 40 km x 240 km.
Both forward- and back-scan pixels are generally processed and written to the products.

5.4 Delivery Time

DLR generates near-real-time (NRT), off-line (OL), and reprocessed products. The NRT products are available for distribution in less than 15 minutes after the reception of the GOME level 0 or level 1 product.

Assuming that the input data is received at DLR 1:45 hours after sensing, then the GOME total column products will be disseminated to the users in less than 2 hours after sensing.
The GOME-2/MetOp OL products are available two weeks after sensing. The GOME/ERS-2 OL products are available up to four weeks after sensing due to constraints on the current level 0 data dissemination.
Based on the experience with GOME/ERS-2, it is expected that level 2 products reprocessed with improved algorithms will be available every two to three years.

5.5 Expected Accuracy

The following table lists the GOME total column trace gases and cloud products provided by DLR together with estimated uncertainties.

Product	*Acronym*	*Expected Accuracy*	*Expected Precision*
Total ozone column	O3	3.6-4.3% (SZA < 80°) 6.4-7.2% (80° < SZA < 90°)	2.4-3.3% (SZA < 80°) 4.9-5.9% (80° < SZA < 90°)
Tropospheric ozone column	O3Tropo	20-40%	20-40%
Total NO_2 column	NO2	5-10% (unpolluted conditions)	3-10% (unpolluted conditions)
Tropospheric NO_2 column	NO2Tropo	50-100% (polluted conditions) > 100% (unpolluted)	50-100% (polluted conditions) > 100% (unpolluted)
Total BrO column	BrO	20-50%	10-50%
Total H_2O column	H2O	5-20%	10-25%
Total SO_2 column	SO2	50-100% (SZA < 70°) >100% (SZA > 70°)	20-50% (SZA < 70°) >50% (SZA > 70°)
Total HCHO column	HCHO	50-100% (polluted conditions) > 100% (unpolluted)	20-50% (polluted conditions) > 100% (unpolluted)
Total OClO column	OClO	50-100% (SZA > 75°)	20-50% (SZA > 75°)
Cloud fraction	CF	< 10%	< 10%
Cloud-top height (pressure)	CTH (CTP)	< 10%	< 10%
Cloud-top albedo (optical thickness)	CTA (COT)	< 10%	< 10%

The algorithms used for NRT and OL processing are the same; this means that NRT and OL products have the same accuracy and precision.

5.6 Product Formats

The format of the product file is either HDF5 or BUFR. A detail description of the HDF5 product format is given in section 6 on page 23, and for the BUFR product in section 7 on page 37.

5.7 File Name

The file name of a product already contains important information about the dataset including trace gases and sensing time. It is built according to the following structure:

SENSOR_GAS_LV_YYYYMMDDhhmmss_ddd_MISSION_#####_PRO_RV.TYPE

where

- *SENSOR* denotes the instrument, i.e. GOME
- *GAS* is a "-" separated list of trace gases included in the product. The acronyms from the above table are used, e.g. "O3-NO2-BrO" is a products containing these three trace gases.
- *LV* is the product level, i.e. L2
- *YYYYMMDD* are the year, month and day of the first processed ground pixel
- *hhmmss* are the hours, minutes and seconds of the UTC time stamp of the first processed ground pixel
- *ddd* is the three digit duration of the product in minutes
- MISSION denotes the mission: ERS2, METOPA, METOPB, METOPC
- *#####* is the five digit orbit number
- *PRO* is the processing center, i.e. DLR
- *RV* is the two digit product revision
- *TYPE* denotes the product format used: HDF5 or BUFR

For example, the following identifier denotes a GOME/ERS-2 off-line product:

GOME_O3-NO2_L2_20060723165752_023_ERS2_58855_DLR_05.HDF5

The following example is a valid name for a GOME-2/MetOp off-line product:

GOME_O3-NO2-BrO_L2_20070302111155_047_METOPA_01900_DLR_01.HDF5

Note: The GOME-2/MetOp NRT products disseminated via EUMETCast have a fixed prefix file name: S-O3M_, see the following example:

S-O3M_GOME_O3_L2_20070302111155_003_METOPA_01900_DLR_01.BUFR

5.8 Product Dissemination

5.8.1 GOME/ERS-2

GOME/ERS-2 products are available at the D–PAF FTP–server:

ftp-ops.de.envisat.esa.int

The OL products are organized in directories as follows:

products/level_2_HDF5/*YYYY*/*MM*/*DD*

where *YYYY* is the year, *MM* the month, *DD* the day.

The NRT products are available in the above D-PAF FTP-server and are organized in the same way as the off–line products, but they are located in the directory *nrt_products*.

5.8.2 GOME-2/MetOp

The primary dissemination mean of GOME-2/MetOp NRT products is EumetCast using the BURF and HDF5 format.

On request, the NRT and OL products are directly pushed to dedicated FTP servers located at the user's premises.

Additionally the GOME-2/MetOp NRT and OL products in HDF5 format are available at the DLR WDC FTP–server:

wdc.dlr.de

under the links "Data & Products" -> "Trace Gases".
The OL products are organized in directories as follows:

products/level_2_HDF5/YYYY/MM/DD

where

- *YYYY* is the year
- *MM* is the month
- *DD* is the acquisition day

In a similar way the NRT products are located in the directory *nrt_products*.

5.9 Product Ordering

5.9.1 GOME/ERS-2

GOME/ERS-2 total column products are generated at DLR's D-PAF on behalf of ESA. For ordering/registration please contact:

ESA ESRIN - EO Help Desk
eohelp@esa.int

Current and historical quicklook images as well as value added products generated by DLR are available at:

http://wdc.dlr.de/sensors/gome

5.9.2 GOME-2/MetOp

The GOME-2/MetOp total column products are generated at DLR in the framework of EUMETSAT's O3M-SAF. For information and access to all O3M-SAF products, please refer to the O3M-SAF help desk:

O3M-SAF Helpdesk
o3msaf@fmi.fi

Additional information can be found in EUMETSAT's product Navigator accessible through the following link:

http://navigator.eumetsat.int

Current and historical quicklook images as well as value added products generated by DLR are available at:

http://wdc.dlr.de/sensors/gome2

6 HDF5 Product Format Description

The product content comprises the following groups:

- *META_DATA*
  - Product Metadata
- *GEOLOCATION*
  - Date & Time (all retrievals)
  - 4 Corner Coordinates & Centre of Ground Pixel
  - Solar, Line-of-Sight Zenith, and relative Azimuth angles at TOA
  - Orbit information
- *TOTAL_COLUMNS*
  - Total and tropospheric column amounts of the various trace gases with corresponding (relative) errors
- *CLOUD_PROPERTIES*
  - Retrieved cloud properties
- *DETAILED_RESULTS*
  - Geophysical parameters (surface, cloud and aerosol values)
  - Vertical column, slant column, ghost column and AMF values with corresponding errors
  - Fitting diagnostics (chi-square, RMS, etc.)
  - Various subgroups for trace gas specific data (e.g. O3, NO2Tropo, SO2)

6.1 Structure

The data in the HDF5 file is organized in five groups: *META_DATA*, *GEOLOCATION*, *TOTAL_COLUMNS*, *DETAILED_RESULTS*, *CLOUD_PROPERTIES (Figure 3).* The values in all groups are either copied from the level 1 ([R4], [R5]) or other input data, or calculated by the UPAS level 1-to-2 processor. The *META_DATA* group contains parameters required by EECF [A2] or UMARF [A3], and general information about the product. The data related to each ground pixel is divided into three groups: *GEOLOCATION*, *TOTAL_COLUMNS* and *DETAILED_RESULTS*. The *GEOLOCATION* group contains all information related to geolocation of the pixel. Pixel processing information is stored in the *TOTAL_COLUMNS* and *DETAILED_RESULTS* groups. Cloud properties derived are stored in the CLOUD_PROPERTIES group.
The last three groups mentioned above contain all pixel information, stored in arrays with length equal to the number of ground pixels in one granule (orbit or PDU). Data values may occur more than once for a given ground pixel, and these will be separated by fitting windows. The information for each entry is stored as a matrix. Elements in these matrices are not always atomic: they can contain variable length data structures. When entries for a pixel or pixel-window combination cannot be calculated using the normal processing procedure, “fill-in” values are written to the arrays. Also, not all datasets defined here have to exists in every product.
Please note that this description is only valid for the actual version of the product format, currently 2/A. The version of a GOME HDF5 level 2 product can reliably be read from the field *META_DATA/ProductFormatVersion*, therefore a reader can implement several versions in parallel.

Each array has five attributes: *Title*, *Unit*, *FillValue*, *ValueRangeMin* and *ValueRangeMax* (Figure 3). These are used to describe the contents of the array.
Values in the *META_DATA* group are stored as attributes of the group.

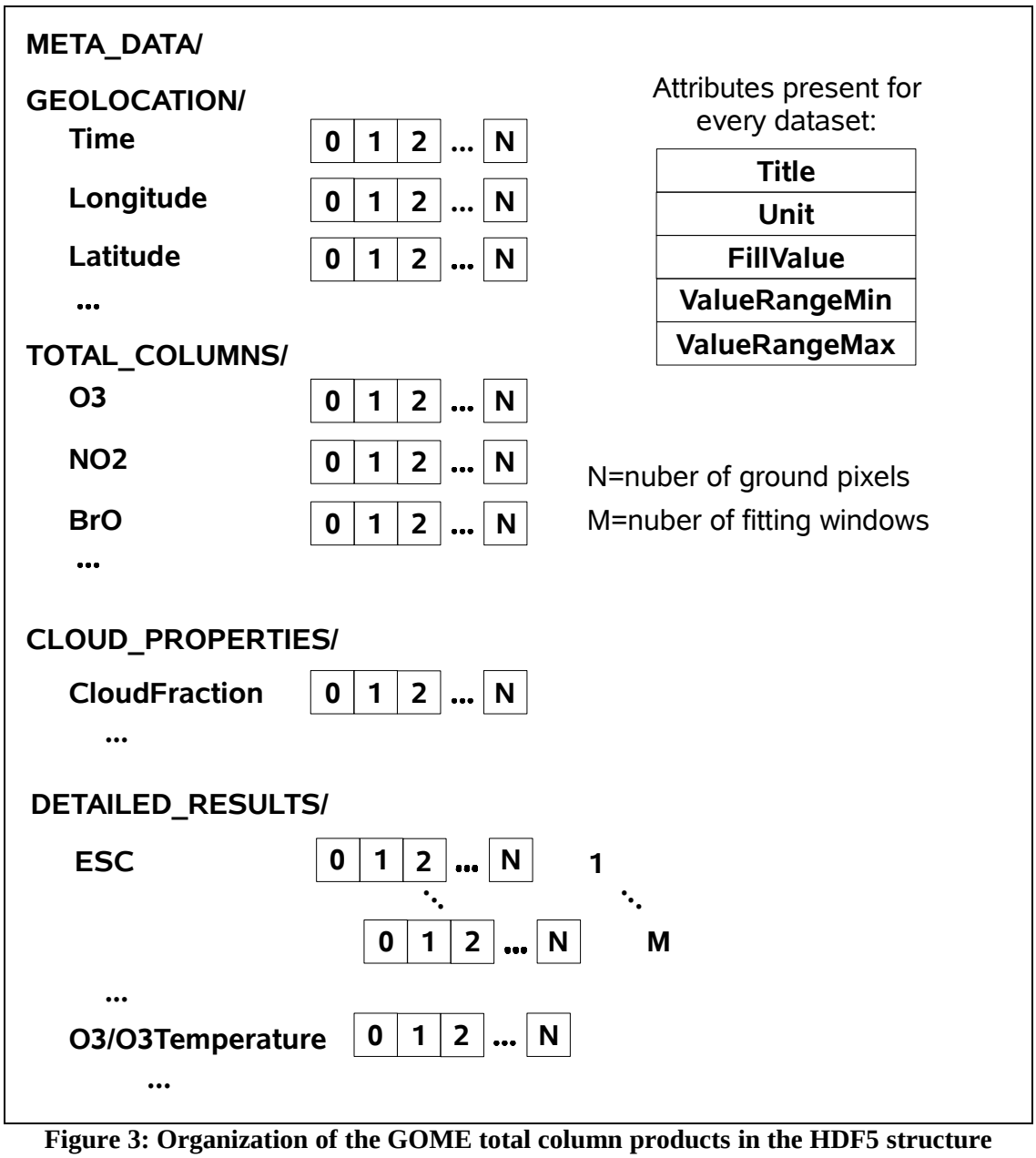


Figure 3: Organization of the GOME total column products in the HDF5 structure

6.1.1 Description of Common Items

In the *GEOLOCATION* and *TOTAL_COLUMN* groups, all datasets have a set of attached attributes. These are shown in the table below.

Attribute Name	*Data Type*	*Description*
Title	string	Description of the dataset, e.g. “Ozone total column”
Unit	string	Unit of the values in the array, e.g. “DU”
FillValue	same as dataset	Value in the array, if actual data value is missing
ValueRangeMin	same as dataset	Minimum value in this dataset (present only when applicable)
ValueRangeMax	same as dataset	Maximum value in this dataset (present only when applicable)

6.2 *META_DATA* Group

The content of the *META_DATA* group is shown in the following tables. Allowed values for parameters required by EECF and UMARF are consistent with requirements given in [A2] and [A3]. Allowed values specified in italics indicate any value of the given type (e.g. *string* means that the attribute can contain any string within the UMARF size limit)

Attribute Name	*Data Type*	*Description*	*Allowed Values GOME/ERS-2*	*Allowed Values GOME-2/Metop*
ArchiveFacility	string	Centre where the data is archived.	D-PAF DLR OP	O3DLR
SatelliteID	string	Platform identifier (mission and spacecraft).	ERS-2	M*nn*
StartOrbitNumber	integer	Orbit number at the start of sensing, i.e. at the beginning of a dump.	*integer*	*integer*
InstrumentID	string	Instrument which acquired the product	GOME	GOME
InstrumentMode	VIEW_MODES structure	Specifies how many ground pixels were observed in the corresponding view modes.	*VIEW_MODES structure*	*VIEW_MODES structure*
SensingStartTime	CCSDS_ASCII	UTC date and time at sensing start.	*Date in CCSDS format (ASCII)*	*Date in CCSDS format (ASCII)*
SensingEndTime	CCSDS_ASCII	UTC date and time at sensing end.	*Date in CCSDS format (ASCII)*	*Date in CCSDS format (ASCII)*
ReceivingCentre	string	Centre that received the data.	KS, GS, DP, ES, MS	ECF (for EECF), FBK, FUC, GCA, PGS, RUS, SOC, SVL, UBI, WAL, WEC, WIV
ProcessingCentre	string	Centre that generated the data.	D-PAF DLR OP	O3DLR
ProcessingMode	string	Processing mode applied for generation of the product.	N (nominal), B (backlogged), R (reprocessed), V (validation) T (near-real-time)	N (nominal), B (backlogged), R (reprocessed), V (validation) T (near-real-time)
Revision	string	Global product revision, required e.g. for reprocessing, part of logical product identifier.	*string*	*string*
ProductType	string	Description of the product type	ERSNTO, ERSOTO	O3MNTO, O3MOTO

Attribute Name	*Data Type*	*Description*	*Allowed Values*
ProcessingLevel	string	Processing level applied for generation of the product.	02
ProcessingTime	CCSDS_ASCII	UTC date and time at processing finish.	CCSDS Date
BaseProductAlgorithmVersion	string	Version of the algorithm used to generate the L1B parent product upon which the L2 product is based.	string
BaseProducts	string	Name of the base products.	string
ProductAlgorithmVersion	string	Version of the algorithm that produced the product.	string
InitializationFileVersion	string	Version of the configuration file used for processing.	string
InternalProcessorRevision	string	Version of the processor used to generate this product.	string
ProductFormatType	string	Data format of the product.	“HDF5”
ProductFormatVersion	string	Version number of the product format.	string
ProductContents	string	Trace gases included in the product (comma-separated list).	string
SubsettingRegion	string	Description of the sub setting region. “full” means: no subsisting was applied.	string
SubSatellitePointStartLat	float	Latitude of the sub-satellite point at start of acquisition. (For EPS products: either the first measurement or first complete scan start point (tbd), at start of dataset.)	-90... 90
SubSatellitePointStartLon	float	Longitude of the sub-satellite point at start of acquisition.	0... 360
SubSatellitePointEndLat	float	Latitude of the sub-satellite point at end of acquisition.	-90... 90
SubSatellitePointEndLon	float	Longitude of the sub-satellite point at end of acquisition.	0... 360
SatellitePosition	POS_VEC	Position vectors (X,Y,Z) in km	Vector in POS_VEC
SatelliteVelocity	POS_VEC	Velocity vector (dx/dt, dy/dt, dz/dt) in km/s	Vector in POS_VEC
OrbitSemiMajorAxis	float	Semi-major axis (km)	float
OrbitExcentricity	float	Excentricity	float
OrbitInclination	float	Inclination (deg)	float
OrbitRightAscOfAscNode	float	Right asc. of asc. node (deg)	float
OrbitArgumentOfPerigee	float	Argument of perigee (deg)	float
OrbitMeanAnomaly	float	Orbit mean anomaly (deg)	float
OrbitUTCDaysSince1950	integer	UTC days since 1.1.1950	int
OrbitMsSinceMidnight	integer	UTC ms since midnight	int
OrbitAscendingNodeCrossing DateTime	CCSDS_ASCII	Ascending node crossing UTC date and time	CCSDS Date
OrbitAscendingNodeLongitude	float	Ascending node longitude	-180... 180 (UMARF notation)
OrbitActualDuration	integer	Orbit duration in minutes, only counting valid pixels	0...~60
SolarSpectraDate	CCSDS_ASCII	Date and time of the solar spectra	CCSDS Date
NumberOfGroundPixels	integer	Number of ground pixels in the product	int
DegradedRecordCount	integer	Number of records which could not be processed by the software.	int
DegradedRecordPercentage	integer	Percentage of records, which could not be processed by the software.	0-100%
MissingDataCount	integer	Number of missing data records.	int
MissingDataPercentage	integer	Percentage of missing data records.	0-100%

The next table contains metadata specific to the total column products.

Attribute Name	*Data Type*	*Description*	*Allowed Values*
NumberOfFittingWindows	integer	Number of fitting windows used in processing	1- M
FittingFlag	integer	Flag indexing DOAS fitting algorithm settings	bitmap
AMFFlag	integer	Flag indexing AMF algorithm settings	bitmap
VCDFlag	integer	Flag indexing VCD algorithm settings	Bitmap

This table describes data sets containing information about the fitting windows:

Dataset Name	*Data Type*	*Description*	*Allowed Values*
FWName	string[windows]	Names of fitting windows	string
FWLowerBound	float[windows]	Lower wavelength bound of a fitting window in nm	240-780
FWUpperBound	float[windows]	Upper wavelength bound of a fitting window in nm	240-780
MainSpecies	string[windows]	Name of the main reference species retrieved in this fitting window	string
VCDQualityIndicator	float[windows]	Percentage of flagged pixels (see QualityFlags 0-2 in 6.7.1) for this window	0-100%

6.3 *GEOLOCATION* Group

The *GEOLOCATION* group contains information for seven different points for the ground **pixel**, denoted by letters A to G in Figure 4.

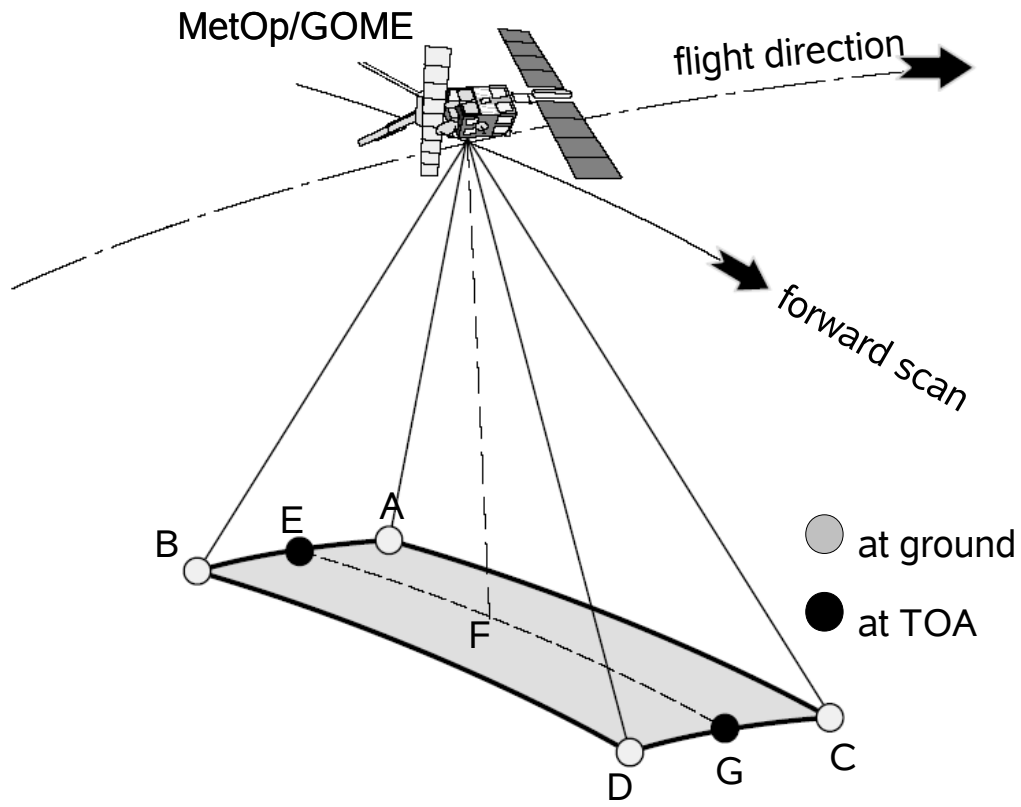


Figure 4: Ground Pixel Geometry

The data sets in the *GEOLOCATION* group are given in the following table:

Dataset Name	*Data Type*	*Unit*	*Description*
InternalPixelId	integer[pixels]	-	Internal ground pixel number
Time	UTC[pixels]	ms	Time of the observation in UTC format
LongitudeCentre	float[pixels]	degrees	Longitude of the centre of the ground pixel (F)
LatitudeCentre	float[pixels]	degrees	Latitude of the centre of the ground pixel (F)
LongitudeA	float[pixels]	degrees	Longitude (A)
LatitudeA	float[pixels]	degrees	Latitude (A)
LongitudeB	float[pixels]	degrees	Longitude (B)
LatitudeB	float[pixels]	degrees	Latitude (B)
LongitudeC	float[pixels]	degrees	Longitude (C)
LatitudeC	float[pixels]	degrees	Latitude (C)
LongitudeD	float[pixels]	degrees	Longitude (D)
LatitudeD	float[pixels]	degrees	Latitude (D)
SolarZenithAngleE	float[pixels]	degrees	Solar zenith angle at TOA (E)
SolarZenithAngleCentre	float[pixels]	degrees	Solar zenith angle at TOA (F)
SolarZenithAngleG	float[pixels]	degrees	Solar zenith angle at TOA (G)
LineOfSightZenithAngleE	float[pixels]	degrees	Line-of-sight zenith angle at TOA (E)
LineOfSightZenithAngleCentre	float[pixels]	degrees	Line-of-sight zenith angle at TOA (F)
LineOfSightZenithAngleG	float[pixels]	degrees	Line-of-sight zenith angle at TOA (G)
RelativeAzimuthE	float[pixels]	degrees	Relative azimuth at TOA (E)
RelativeAzimuthCentre	float[pixels]	degrees	Relative azimuth at TOA (F)
RelativeAzimuthG	float[pixels]	degrees	Relative azimuth at TOA (G)
SolarZenithAngleSatE	float[pixels]	degrees	Solar zenith angle at satellite (E)
SolarZenithAngleSatCentre	float[pixels]	degrees	Solar zenith angle at satellite (F)
SolarZenithAngleSatG	float[pixels]	degrees	Solar zenith angle at satellite (G)
LineOfSightZenithAngleSatE	float[pixels]	degrees	Line-of-sight zenith angle at satellite (E)
LineOfSightZenithAngleSatCentre	float[pixels]	degrees	Line-of-sight zenith angle at satellite (F)
LineOfSightZenithAngleSatG	float[pixels]	degrees	Line-of-sight zenith angle at satellite (G)
RelativeAzimuthSatE	float[pixels]	degrees	Relative azimuth at satellite (E)
RelativeAzimuthSatCentre	float[pixels]	degrees	Relative azimuth at satellite (F)
RelativeAzimuthSatG	float[pixels]	degrees	Relative azimuth at satellite (G)
SubSatellitePointLongitude	float[pixels]	degrees	Geodetic longitude of subsatellite point
SubSatellitePointLatitude	float[pixels]	degrees	Geodetic latitude of subsatellite point
SatelliteAltitude	float[pixels]	km	Geodetic altitude of satellite
EarthRadius	float[pixels]	km	Radius of the Earth
IndexInScan	integer[pixels]	-	Index of the pixel within the scan (0-3)
SubPixelInScan	integer[pixels]	-	Subpixel within the scan (0-3 for GOME/ERS-2; 0 to 3, 7 or 31 for GOME-2/MetOp)
ViewMode	string[pixels]	Nominal, NorthPolar, SouthPolar, Narrow, Static	Scanning mode of the instrument at the time of acquisition
PixelFlag (future use)	integer[pixels]	-	Flag for different pixel retrieval conditions, e.g. land/sea, sun glint or snow/ice

6.4 *TOTAL_COLUMNS* Group

The data sets in the *TOTAL_COLUMNS* group are given in the following tables. Attributes attached to all data sets in this group are the same as those for the *GEOLOCATION* group.
This group contains the key trace gas total column information. Data sets are arrays of size N, where N is the number of ground pixels in the product granule.
All entries starting with the name of the trace gas are only included if the trace gas total column has been retrieved, in which case it is included in the /META_DATA/MainSpecies attribute.

Dataset Name	*Data Type*	*Unit*	*Description*
O3	float[pixels]	Dobson Units	Total vertical column density of O3
O3_Error	float[pixels]	%	Error on total vertical column density of O3
O3Tropo (*)	float[pixels]	Dobson Units	Tropospheric vertical column density of O3
O3Tropo_Error (*)	float[pixels]	%	Error on tropospheric vertical column density of O3
O3Tropo_Flag (*)	float[pixels]	-	Flag indexing tropospheric O3 calculation
NO2	float[pixels]	molecules/cm2	Vertical column density of NO2
NO2_Error	float[pixels]	%	Error on vertical column density of NO2
NO2_Corr	float[pixels]	molecules/cm2	Total vertical column density of NO2 corrected for tropospheric contribution
NO2_Corr_Error (*)	float[pixels]	%	Error on corrected total vertical column density of NO2
NO2Tropo	float[pixels]	molecules/cm2	Tropospheric vertical column density of NO2
NO2Tropo_Error (*)	float[pixels]	%	Error on tropospheric vertical column density of NO2
NO2Tropo_Flag	float[pixels]	-	Flag indexing tropospheric NO2 calculation (see 6.7.2)
BrO (*)	float[pixels]	molecules/cm2	Vertical column density of BrO
BrO_Error (*)	float[pixels]	%	Error on vertical column density of BrO
BrO_Corr (*)	float[pixels]	molecules/cm2	Total vertical column density of BrO corrected for tropospheric contribution
BrO_Corr_Error (*)	float[pixels]	%	Error on corrected total vertical column density of BrO
BrOTropo (*)	float[pixels]	molecules/cm2	Tropospheric vertical column density of BrO
BrOTropo_Error (*)	float[pixels]	%	Error on tropospheric vertical column density of BrO
BrOTropo_Flag (*)	float[pixels]	-	Flag indexing tropospheric BrO calculation
H2O (*)	float[pixels]	molecules/cm2	Vertical column density of H2O
H2O_Error (*)	float[pixels]	%	Error on vertical column density of H2O
OClO (*)	float[pixels]	molecules/cm2	Vertical column density of OClO
OClO_Error (*)	float[pixels]	%	Error on vertical column density of OClO
SO2	float[pixels]	Dobson Units	Vertical column density of SO2
SO2_Error	float[pixels]	%	Error on vertical column density of SO2
HCHO (*)	float[pixels]	molecules/cm2	Vertical column density of HCHO
HCHO_Error (*)	float[pixels]	%	Error on vertical column density of HCHO

(*) for future use, not yet implemented

6.5 *CLOUD_PROPERTIES* Group

In this group, the main cloud properties of each pixel are stored.

Dataset Name	*Data Type*	*Unit*	*Description*
CloudFraction	float[pixels]	-	Cloud fraction
CloudFraction_Error	float[pixels]	%	Error on cloud fraction
CloudTopAlbedo	float[pixels]	-	Cloud-top albedo (-1 if clear sky)
CloudTopAlbedo_Error	float[pixels]	%	Error on cloud-top albedo (-1 if clear sky)
CloudTopHeight	float[pixels]	km	Cloud-top height (-1 if clear sky)
CloudTopHeight_Error	float[pixels]	%	Error on cloud-top height (-1 if clear sky)
CloudOpticalThickness	float[pixels]	-	Cloud optical thickness (-1 if clear sky)
CloudOpticalThickness_Error	float[pixels]	%	Error on cloud optical thickness (-1 if clear sky)
CloudTopPressure	float[pixels]	hPa	Cloud-top pressure (-1 if clear sky)
CloudTopPressure_Error	float[pixels]	%	Error on cloud-top pressure (-1 if clear sky)
CloudType	integer[pixels]	-	ISCCP cloud type classification (-1 if clear sky): 1 = cirrus, 2 = cirrostratus, 3 = deep convection, 4 = altocumulus, 5 = altostratus, 6 = nimbostratus, 7 = cumulus, 8 = stratocumulus, 9 = stratus
CloudMode	integer[pixels]	-	Mode in which cloud parameters have been calculated 0=normal mode, 1=snow/ice mode
SurfaceAlbedo	float[pixels]	-	Surface albedo used for cloud retrieval

6.6 *DETAILED_RESULTS* Group

The following table lists ancillary surface/aerosol data and detailed processing results, as stored in the *DETAILED_RESULTS* group. Data sets (see Figure 3 on page 25) are represented either as arrays of size N, where N is the number of ground pixels in the product, or as matrices of dimensions NxM, for N the number of ground pixels (denoted as "pixels" in the following tables) and M the number of fitting windows (denoted as "windows" in the following tables).

Dataset Name	*Data Type*	*Unit*	*Description*
AAI	float[pixels]	-	Absorbing aerosol indicator
SurfaceHeight	float[pixels]	km	Surface altitude
SurfacePressure	float[pixels]	hPa	Pressure at the surface level
SurfaceAlbedoRW	float[pixels][windows]	-	Surface albedo for the associated retrieval window
VCD	float[pixels][windows]	mol/cm^2	Vertical column density of main parameter value
VCD_Error	float[pixels][windows]	%	Error on vertical column density
IntensityWeightedCloudFraction	float[pixels][windows]	-	Weighting factor between clear-sky and cloudy AMFs
ESC	float[pixels][windows]	mol/cm^2	Retrieved effective slant column
ESC_Error	float[pixels][windows]	%	Error on effective slant column
FittingRMS	float[pixels][windows]	-	RMS of the fit
FittingChiSquare	float[pixels][windows]	-	Square of Chi
FittingGoodness	float[pixels][windows]	-	Goodness of fit for the fitting window
FittingNumberOfIterations	integer[pixels][windows]	-	Number of iterations of non-linear fitting
GhostColumn	float[pixels][windpws]	mol/cm^2	Ghost column used in VCD
AMFToGround	float[pixels][windows]	-	AMF to ground for species
AMFToGround_Error	float[pixels][windows]	%	Error on AMF to ground
AMFToCloudTop	float[pixels][windows]	-	AMF to cloud-top for species (-1 if clear sky)
AMFToCloudTop_Error	float[pixels][windows]	%	Error on AMF to cloud-top (-1 if clear sky)
AMFTotal	float[pixels][windows]	-	Total AMF
AMFTotal_Error	float[pixels][windows]	%	Total AMF error
QualityFlags	integer[pixels][windows]	-	Quality flags for each pixel/window (see 6.7.1)

The following subsections contain sub groups of the *DETAILED_RESULTS* group which contain trace gas specific data.

6.6.1 *DETAILED_RESULTS/O3* Subgroup

In the following table, the number of atmospheric layers is denoted as “layers” in profile datasets.

Dataset Name	*Data Type*	*Unit*	*Description*
ESCRingCorrected	float[pixels]	mol/cm^2	Retrieved effective slant column (ring-corrected for ozone)
O3Temperature	float[pixels]	K	Fitted ozone temperature
RingCorrection	float[pixels]	-	Applied ring correction factor
O3Profile	float[pixels][layers]	DU	A priori O_3 profile used in the retrieval of O_3 (layers=13, optional parameter)
TemperatureProfile	float[pixels][layers]	K	A priori temperature profile used in the retrieval of O_3 (layers=13, optional parameter)
IterativeVCDNumberOfIterations	integer[pixels]	-	Number of iterations for the iterative VCD algorithm

6.6.2 *DETAILED_RESULTS/NO2* Subgroup

Dataset Name	*Data Type*	*Unit*	*Description*
AMFTropoToGround	float[pixels]	-	Tropospheric AMF for cloud-free part
AMFTropoToGround_Error	float[pixels]	%	Error on Tropospheric AMF for cloud-free part
AMFTropoToCloudTop	float[pixels]	-	AMF for cloudy part (-1 if clear sky)
AMFTropoToCloudTop_Error	float[pixels]	%	Error on AMF for cloudy part (-1 if clear sky)
AMFTropo	float[pixels]	-	Tropospheric AMF
AMFTropo_Error	float[pixels]	%	Error on tropospheric AMF
VCDStrato	float[pixels]	mol/cm^2	Stratospheric vertical column density
VCDStrato_Error	float[pixels]	%	Error on stratospheric vertical column density
VCDTropo	float[pixels]	mol/cm^2	Tropospheric vertical column density
VCDTropo_Error	float[pixels]	%	Error on tropospheric vertical column density
VCDCorrected	float[pixels]	mol/cm^2	Total vertical column density corrected for tropospheric contribution
VCDCorrected_Error	float[pixels]	%	Error on corrected total vertical column density
NO2Tropo_Flag	integer[pixels]	-	Flag indexing tropospheric NO2 calculations (see 6.7.2 on page 36)

6.6.3 *DETAILED_RESULTS/SO2* Subgroup

The SO2 algorithm internally calculates results for several assumed plume heights. The number of plume heights is available in the field "NumberOfPlumeHeigths", which also describes the cardinality of the subsequent datasets (denoted as "heigths"). The different height values are available in the dataset "PlumeHeigths".

Attribute Name	*Data Type*	*Unit*	*Description*
NumberOfPlumeHeights	integer	-	Number of assumed plume heights
Dataset Name	***Data Type***	***Unit***	***Description***
PlumeHeights	float[heights]	km	Assumed plume heights for retrieval
ESCCorrected	float[pixels][heights]	mol/cm^2	Slant column density (background corrected)
AMFToGround	float[pixels][heights]	-	AMF to ground
AMFToGround_Error	float[pixels][heights]	%	Error on AMF to ground
AMFToCloudTop	float[pixels][heights]	-	AMF to cloud-top (-1 if clear sky)
AMFToCloudTop_Error	float[pixels][heights]	%	Error on AMF to cloud-top (-1 if clear sky)
AMFTotal	float[pixels][heights]	-	Total AMF
AMFTotal_Error	float[pixels][heights]	%	Total AMF error
VCDCorrected	float[pixels][heights]	mol/cm^2	Total vertical column density (background corrected)
VCDCorrected_Error	float[pixels][heights]	%	Error on total vertical column density
SO2_Flag	integer[pixels]	-	Flag indexing SO2 calculations (see 6.7.3 on page 36)

6.7 Detailed Flag Description

6.7.1 QualityFlags

Flag	*Value*	*Description*	*Specified Valid Conditions*			
			O3	*NO2*	*BrO*	*SO2*
0	1	**Invalid total column** If the retrieved total column is invalid, it is replaced with the fill value and this flag is set, together with flags 1 and 2	retrieval possible and result >= 0	retrieval possible	retrieval possible	retrieval possible
1	2	**Total column out of range** Set if the total column retrieved for this ground pixel is outside the specified range	75-700 DU	0-5*10^{16} mol/cm^2	0-1.5*10^{14} mol/cm^2	-10–1000 DU
2	4	**Large error in ESC** Set if the *ESC_Error* value of this ground pixel exceeds the specified threshold	<=2%	<=50%	<=100%	Not applicable

These flags give additional information about the quality of the total column retrieval. If for example the fitting of the slant column does not succeed (or in case of ozone the fitting results produce negative values), flag 0 (and also flag 1 and 2) is set to indicate this condition, and the total column field will contain the fill value.
If the total column has been retrieved, but is out of the specified range, flag 1 is set. If the associated slant column error exceeds a specific threshold, flag 2 is set.
See *VCDQualityIndicator* in 6.2 on page 26 for the percentage of pixels which have been flagged as an overall quality indicator for the whole orbit.

6.7.2 NO2Tropo_Flag

Flag	*Value*	*Description*
0	1	***Polluted condition**: NO2Tropo* and *NO2_Corr* values are available. ● *NO2* contains the total column density based on an unpolluted AMF. ● *NO2_Corr* contains the pollution corrected total column density. ● *NO2Tropo* contains the tropospheric column density. Note: *IntensityWeightedCloudFraction* < 50%
1	2	***Unpolluted condition***: *NO2Tropo* and *NO2_Corr* not available (fill-values). ● *NO2* contains the total column density based on an unpolluted AMF. Note: *IntensityWeightedCloudFraction* < 50%.
2	4	***Cloudy condition***: *NO2Tropo* and *NO2_Corr* not available (fill-values). ● *NO2* contains the total column density based on an unpolluted AMF. Note: *IntensityWeightedCloudFraction* > 50%
3	8	***Measurement in polar regions*** (Lat > 70 deg): *NO2Tropo* and *NO2_Corr* not available (fill-values). ● *NO2* contains the total column density based on an unpolluted AMF
4	16	***NO2 column data not available***: ● *NO2*, *NO2Tropo* and *NO2_Corr* contain fill-values

6.7.3 SO2_Flag

Flag	*Value*	*Description*
0	1	***Measurement in polar regions*** (SZA > 75 deg): ● reduced quality of SO2 total column
1	2	***SO2 column data not available***: ● *SO2* and S*O2_Corr* contain fill-values

7 BUFR Product Format Description

7.1 Structure

The data in the BUFR file is organized in six sections: *INDICATOR SECTION*, *IDENTIFICATION*, *OPTIONAL SECTION*, *DATA DESCRIPTION*, *DATA SECTION* and *END SECTION*. The values in all sections are either copied from the level 1 ([R4], [R5]) or other input data, or calculated by the level 1-to-2 processor. Each of the sections of a BUFR message is made up of a series of octets. The term octet, meaning 8 bits, was coined to avoid having to continually qualify byte as an 8-bit byte.
The *DATA DESCRIPTION* section contains a list of descriptors defining the structure and the format of data following in *DATA SECTION*. This is called "self-descriptive" nature of BUFR. The strength of this self-descriptive feature is in accommodating change. For example, if new observations or observational platforms are developed, there is no need to invent a new code form to represent and transmit the new data; all that is necessary is the publication of additional data description tables. Similarly for the deletion of possibly outdated observations: instead of having to send "missing" indicators for a long period while awaiting a change to a fixed format code, the "missing" data are simply not sent in the message and the data description section is adjusted accordingly. The data description tables are not changed, however, so that archives of old data may be retrieved.
The data encoded in BUFR format is purely binary or bit oriented, thus making it both machine dependent and, at the same time, machine independent. The dependency comes in the construction or interpretation of BUFR messages: there is not much for a human to look at as all the numbers in a message, whether data descriptors or the data themselves, are binary integers. And that, of course, leads to the machine independence: with BUFR consisting entirely of binary integers any brand of machine can handle BUFR as well as any other.
Theoretically there is no upper limit to the size of a BUFR message but, by convention, BUFR messages are restricted to 15000 octets or 120000 bits. This limit is to allow an entire BUFR message to be contained within memory of most computers for decoding. It is also a limit set by the capabilities of the Global Telecommunications System (GTS) of the WMO. In UPAS the length of a single BUFR message is limited to 200 ground pixels, that gives approximately 10Kbytes for storing one message. The file contains the information corresponding to a single orbit can contain unlimited number of consecutive BUFR messages.

7.2 Section 0 - Indicator Section

Octet	*Description*	*Allowed Values*
1-4	"BUFR" (coded according to the CCITT International Alphabet No. 5)	"BUFR"
5-7	Total length of BUFR message, in octets (including Section 0)	0-15000
8	BUFR edition number (currently 4)	1-4

7.3 Section 1 - Identification Section

Octet	*Description*	*Allowed/Used Values*
1-3	Length of section, in octets	int value
4	BUFR master table (zero if standard WMO FM 94 BUFR tables are used - provides for BUFR to be used to represent data from other disciplines, and with their own versions of master tables and local tables)	0
5-6	Originating centre: code table 0 01 031	210
7-8	Originating sub-centre	0
9	Update sequence number (zero for original BUFR messages; incremented for updates)	1
10	Bit 1 = 0 No optional section = 1 Optional section included Bits 2 - 8 set to zero (reserved)	0
11	Data Category type (BUFR Table A)	3
12	Data Category sub-type (defined by local ADP centres)	255
13	Local data sub-category	206
14	Version number of master tables used (currently 2 for WMO FM 94 BUFR tables)	11
15	Version number of local tables used to augment the master table in use	0
16-17	Year	2xxx
18	Month	1-12
19	Day	1-31
20	Hour	0-23
21	Minute	0-59
22	Second	0-59

7.4 Section 3 - Indicator Section

Octet	*Description*	*Allowed/Used Values*
1-3	Length of section, in octets	
4	Set to zero (reserved)	
5-6	Number of data subsets	200
7	Bit 1 = 1 observed data = 0 other data Bit 2 = 1 compressed data = 0 non-compressed data Bit 3 - 8 set to zero (reserved)	192
8-	A collection of descriptors which define the form and content of individual data elements comprising one data subset in the data section.	

7.5 Section 3 - UPAS Level-2 Specific List of Descriptors

Descriptor	*Description*	*Value*
0 01 007	Satellite Identifier	5 = Metop-2
0 02 019	Satellite Instruments	220 = GOME-2
3 01 011	Date in format YYYY-MM-DD (0 04 001, 0 04 002, 0 04 003)	
3 01 013	Time in format HH-MM-SS (0 04 004, 0 04 005, 0 04 006)	
3 01 021	Latitude / Longitude Centre (0 05 001, 0 06 001)	
1 02 004	Repeat next 2 fields 4 times (for four corners of a pixel)	
0 27 001	Latitude (High Accuracy)	
0 28 001	Longitude (High Accuracy)	
0 10 001	Height of land surface	
0 14 019	Surface Albedo	0.0-1.0
0 07 025	Solar zenith angle	
0 10 080	Viewing Zenith Angle	
0 05 023	Sun to satellite azimuth difference	
0 20 010	Cloud Cover	[%]
0 08 003	Vertical significance	2 = Cloud top
0 07 004	Pressure	[pa]
0 14 026	Albedo at the top of clouds	0.0-1.0
0 20 014	Height of top of clouds	[km]
0 13 093	Cloud optical thickness	
0 31 001	Delayed descriptor replication factor	2
0 07 004	Pressure	Top
0 07 004	Pressure	Bottom
0 08 043	Atmospheric chemical or physical constituent type	see table below
0 08 044	CAS registry number	see table below
0 15 021	Integrated mass density	[kg/m^2]
2 24 000	First order statistics follow	
2 36 000	Backward reference bitmap	
0 31 001	Delayed descriptor replication factor	2
0 31 031	Data present indicator	0/1
0 01 031	Identification of originating/generating centre	254 (Eumetsat)
0 01 032	Generating Application	1
0 08 023	First order statistics	7 = Mean absolute error
0 31 001	Delayed descriptor replication factor	2
0 15 021	Integrated mass density	[kg/m^2]

7.6 Section 4 - Indicator section.

Octet	*Description*	*Allowed Values*
1-3	Length of section, in octets	
4	Set to zero (reserved)	
5-	Binary data as defined by descriptors which begin at octet 8, Section 3	

7.7 Section 5 - End Section

Octet	*Description*	*Allowed Values*
1-4	"7777" (coded according to the CCITT International Alphabet No. 5)	„7777“

7.8 Trace Gas Table

The following field values are used for the different trace gases:

Trace gas	*Trace gas name*	*Atmospheric Chemical No. (08 043 descriptor)*	*CAS Registry Number (08 044 descriptor)*
O_3	Ozone	0	10028-15-6
NO_2	Nitrogen dioxide	5	10102-44-0
BrO	Bromine oxide	9	15656-19-6
SO_2	Sulfur dioxide	8	7446-09-5
H_2O	Water Vapour	1	7732-18-5
HCHO	Formaldehyde	7	50-00-0
OClO	Chlorine dioxide	10	10049-04-4

A Appendixes

A.1 HDF5 Data Types

The following table shows the correspondence between Product data types and HDF5 data types

Data type	*HDF5 predefined data type*
char	H5T_STD_I8LE
integer	H5T_STD_I32LE
float	H5T_IEEE_F32LE
double	H5T_IEEE_F64LE
string	H5T_C_S1
UTC	H5T_COMPOUND { H5T_STD_I32LE Day, H5T_STD_I32LE MillisecondOfDay }, where Day denotes number of days since 1st of January, 1950

VIEW_MODES	H5T_COMPOUND {
	H5T_STD_I32LE NominalPixels,
	H5T_STD_I32LE StaticPixels,
	H5T_STD_I32LE NarrowPixels,
	H5T_STD_I32LE PolarSouthPixels,
	H5T_STD_I32LE PolarNorthPixels
	}

CCSDS_ASCII	The format for ASCII Time Code is *YYYY-MM-DD*T*hh:mm:ss.ddd*, where: *YYYY* = Year in four-character subfield with values 0001-9999 *MM* = Month in two-character subfield with values 01-12 *DD* = Day of month in two-character subfield with values 01-28,-29, -30, or -31 "T" = Calendar-Time separator *hh* = Hour in two-character subfield with values 00-23 *mm* = Minute in two-character subfield with values 00-59 *ss* = Second in two-character subfield with values 00-59 *ddd* = Decimal fraction of second where each d has values 0-9

POS_VEC	H5T_COMPOUND {
	H5T_IEEE_F64LE X,
	H5T_IEEE_F64LE Y,
	H5T_IEEE_F64LE Z
	}

.

A.2 Traceability Matrix of HDF5 Metadata to EECF Parameters

The EECF metadata parameters [A2] which are applicable to the D-PAF products are stored in the HDF5 file as attributes in the *META_DATA* group. The tracing of EECF parameters to the attributes in the product file is indicated in the following table. Attributes can only take values which are allowed by EECF.

EECF Short Name	*Attribute Name*	*Notes*
SATELLITE_ID	SatelliteID	possible values: ERS; M01, M02... for METOP
SENSOR_ID	InstrumentID	GOME
ORBIT_NO	StartOrbitNumber	
ACQUISITION_FACILITY_ID	ReceivingCentre	ECF, FBK, FUC, GCA, PGS, RUS, SOC, SVL, UBI, WAL, WEC, WIV
PROCESSING_FACILITY_ID	ProcessingCentre +ArchiveFacility	D-PAF DLR OP (ERS), O3DLR (METOP)
PROCESSING_DATE_TIME	ProcessingTime	
TEMPORAL_COVERAGE_START	SensingStartTime	
TEMPORAL_COVERAGE_STOP	SensingEndTime	
SOFTWARE_VERSION	ProductAlgorithmVersion	
AUX_DATA	InitializationFileVersion	
PRODUCT_TYPE	ProcessingLevel	“02” or “03”
REVISION	Revision	
SOURCE_ITEM	BaseProducts	

A.3 Traceability Matrix of HDF5 Metadata to UMARF Parameters

The UMARF metadata parameters [A3] applicable to the O3M-SAF products are stored in the HDF5 file as attributes in the *META_DATA* group. The mapping of UMARF parameters to product file attributes is shown below; again, attributes can only take values allowed by UMARF.

UMARF Short Name	*Attribute Name*	*Notes*
AARF	ArchiveFacility	possible values: D-PAF DLR OP (ERS), O3DLR (METOP)
ABID	ProductContents	Spectral Band Ids
AIID	InstrumentID	GOME
APAS	Applicable (*)	Product Size
APNA	Applicable (*)	Product Name
APNM	ProductType	e.g. O3MOTO, O3MNTO
APPN	BaseProducts	Parent Product Name
ASTI	SatelliteID	possible values: ERS; M01, M02, M03 for METOP
AVBA	BaseProductAlgorithmVersion	
AVPA	ProductAlgorithmVersion	Concatenation of the HDF5 attributes *ProductAlgorithmVersion*, *InitializationFileVersion*, *InternalProcessorRevision*, and *Revision*
GDMD	Applicable (*)	Disposition Mode: T, O, or P
GGTP	Applicable (*)	GranuleType: “DP”
GNFV	ProductFormatVersion	
GORT	Applicable (*)	OrbitType: “LEO”
GPLV	ProcessingLevel	“02” or “03”
GPMD	ProcessingMode	N, B, R, V
LLAE	SubSatellitePointEndLat	-90.0000 to +89.9999
LLAS	SubSatellitePointStartLat	-90.0000 to +89.9999
LLOE	SubSatellitePointEndLon	-180.0000 to +179.9999
LLOS	SubSatellitePointStartLon	-180.0000 to +179.9999
LONS	StartOrbitNumber	
LSVL	OrbitAscendingNodeLongitude	-180.0000 to +179.9999
LSVT	OrbitAscendingNodeCrossingDateTime	CCSDS date
PPRC	ProcessingCentre	possible values: D-PAF DLR OP (ERS), O3DLR (METOP)
PPST	Processing End Date and Time	CCSDS date
QDLC	MissingDataCount	
QDLP	MissingDataPercentage	
QDRC	DegradedRecordCount	
QDRP	DegradedRecordPercentage	
QQAI	Applicable (*)	Associated Quality Information
QQOV	Applicable (*)	Overall quality flag: OK/NOK
RRCC	ReceivingCentre	ECF, FBK, FUC, GCA, PGS, RUS, SOC, SVL, UBI, WAL, WEC,WIV
SMOD	InstrumentMode	e.g. NARROW, NORMAL or STATIC
SNIT	Applicable (*)	CCSDS date
SSBT	SensingStartTime	CCSDS date
SSST	SensingEndTime	CCSDS date

(*) Parameter is not contained in the HDF5 product, but will be provided by DIMS.